

DETAILED OFFICE ACTION

Applicants response filed 06/18/2009 is acknowledged.

Claims 2-5, 7-10, and 12-14 are canceled. Claims 1, 6, and 11 are pending and currently under examination.

Rejections and/or objections not reiterated from previous office actions are hereby withdrawn. The following rejections and/or objections are either reiterated or newly applied. They constitute the complete set presently being applied to the instant application.

Claim Rejections - 35 USC § 101

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 1, 6, and 11 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter. This rejection is newly applied.

The recent en banc decision regarding *Bilski v. Warsaw* (2008) set forth that a process is patent-eligible if (1) it is tied to a particular machine or apparatus or (2) it transforms a particular article into a different state or thing. Further, the recent decision in *Comiskey* (2009) confirmed the opinion set forth in *Bilski* of the prohibition pre-empting an abstract idea or mental process in a claim. The revised *Comiskey* decision further reiterated the precedent set forth in *Richman*, 563 F.2d 1026, 1030 (CCPA 1977)

wherein the court held the application unpatentable because “if a claim [as a whole] is directed essentially to a method of calculating, using a mathematical formula, even if the solution is for a specific purpose, the claimed method is nonstatutory.”

In the instant case, the claims are directed to a method of selecting at least one lead candidate compound. The recited processes comprises the steps of reading three dimensional information of at least one query molecule, selecting lead candidate compounds from a database, estimating a binding scheme, and outputting at least one lead candidate compound. In the instant case, the claims do not recite any transformation of physical article into a different state or thing. Rather, the recited processes is directed abstract manipulations of data. Further, the ultimate outputting step is considered insignificant extra-solution activity because said outputting step does not affect nor is it involved in the critical steps of selecting a lead compound.

Therefore, the examiner must determine if the instant claims are tied to a particular machine or apparatus. It is acknowledged that the preamble has been amended so as to recite “A computer-implemented method”, however said recitation only suggests that a computer may be involved in the process and does not serve to limit the instant claims to any particular machine or apparatus. The actual recited steps that define the claimed process are not limited to any particular machine or field of use. Such a method is not statutory as it would wholly pre-empt the abstract computational process described above.

Response to Arguments

Applicant's arguments filed 06/18/2009 have been fully considered but they are not persuasive.

Applicants argue that the current amendment to the instant claims sufficiently ties them to a particular machine as set forth in *Bilski v. Warsaw*.

Applicants argument is not persuasive for the reasons set forth in the above rejection. Specifically, the recitation of "computer-implemented" only suggests that a computer is somehow used in performing a process. Such a recitation in the preamble fails to provide any meaningful limit to actual process steps recited in the instant claims.

Claim Rejections - 35 USC § 102

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

Claims 1, 6, and 11 are rejected under 35 U.S.C. 102(b) as being anticipated by Wang et al. (IDS ref: J. Med. Chem. (1994) vol. 37, pp. 4479-4489).

The instant claims are drawn to a method for selecting at least one lead-candidate compound capable of binding as a ligand to a protein. The claimed method comprises the steps of inputting at least one query molecule known to bind or expected to be bound by the protein, screening lead-candidate compounds from a compound database by matching modes of covalent bonds between a query and trial compounds

and judging similarities of partial structures of said compounds based on two-dimensional graphs, estimating a binding scheme of the lead-candidate compounds and the query molecule to the protein based on three-dimensional information and outputting at least one lead-candidate compound, and outputting at least one lead-candidate compound capable of binding the protein.

Wang et al. discloses a computer protein kinase C (PK-C) pharmacophore search on 206,876 nonproprietary structures in the NCI 3D-database that led to the discovery of five compounds which were found to possess PK-C binding affinities (see Wang et al., Abstract). Wang et al. disclose the construction of a PK-C pharmacophore query used in the 3D-database pharmacophoric search (see Wang et al., Figure 1) which is known to bind the PK-C receptor (see Wang et al., page 4480 col. 1, lines 1-17). The results of the computer implemented 3D-database pharmacophore search resulted in the identification of 535 that sufficiently matched the PK-C pharmacophore (see Wang et al., page 4480, col. 1, line 18 through col. 2, line 66). Wang et al. further disclose the visual inspection of 286 compounds of the 535 identified matches for the presence of hydrophobic constituents and further displays the 2D structures of 11 of said 286 compounds wherein atoms and covalent bonds are presented (see Wang et al., Figure 2 and page 4480, col. 2, lines 52-66). Wang et al. further disclose the computational molecular modeling study of known PK-C agonists containing a hydrophobic moiety and the use of this information in the qualitative selection of the final 125 compounds (see Wang et al., page 4480, col. 2, line 46-51 and page 4481, col. 2, line 1 through page 4486, col. 2, line 38). Wang et al. further discloses the synthesis

and binding affinity testing of 125 identified compounds (see page 4481, col. 1, lines 1-12). Wang et al further teaches the molecular modeling using the Quanta molecular modeling package (see Wang et al., page 4480, col. 2, lines 46-50) and detailed three-dimensional structure information of the PK-C receptor, lead compounds, and known PK-C agonists structures (see Wang et al., Table 3 and page 4479, col. 2, lines 10, page 4480, col. 1, lines 1-15, page 4482, col. 2, lines 18-41, page 4483, col. 1, line 1 through page 4484, col. 1, line 30). Wang et al. further teaches the estimation of a binding scheme between lead compounds, and known PK-C agonists structures to the PK-C receptor and determined that conformational changes of ligands upon binding on protein receptors do not have to be in their global or local energy minima to bind (see Wang et al., page 4485, col. 1, line 30 through page 4486, col. 1, line 9).

Response to Arguments

Applicants' arguments filed 06/18/2009 have been fully considered but they are not persuasive.

In regard to the rejection of claims under 35 USC § 102(b) as being anticipated by Wang et al., applicants reiterate the argument that Wang et al. does not disclose estimating a binding scheme of the lead-candidate compounds to the protein.

Applicants further reiterate the argument that Wang et al. neither teaches nor suggests how the binding scheme of a lead-candidate compound to a protein may be estimated based on "correspondences of the mode of covalent binding of the partial structures of the query molecule and the trail molecules".

In response, it is reiterated from the instant rejection that Wang et al. further teaches the estimation of a binding scheme between lead compounds to known PK-C agonists structures of the PK-C receptor. These estimated interaction and binding schemes for these compounds are derived from analysis of their three dimensional structures. Wang et al. further teaches the determination that conformational changes of ligands upon binding on protein receptors do not have to be in their global or local energy minima to bind (see Wang et al., page 4485, col. 1, line 30 through page 4886, col. 1, line 9). Contrary to applicants argument, the determination of the effects conformational changes in modeled ligand structures following receptor binding, as taught by Wang et al., reads directly on estimating a binding scheme of lead-candidate compounds to a protein as instantly claimed. Further, the disclosed modeling of ligand conformations upon protein binding by Wang et al. reads directly on a correspondence of the mode of covalent bonds of partial structures of query and trail compounds as instantly claimed. Therefore it is maintained that Wang et al. fully anticipates the claimed invention.

Conclusion

THIS ACTION IS MADE FINAL. Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE MONTHS from the mailing date of this action. In the event a first reply is filed within TWO MONTHS of the mailing date of this final action and the advisory action is not mailed until after the end of the THREE-MONTH shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than SIX MONTHS from the mailing date of this final action.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to ERIC S. DEJONG whose telephone number is (571)272-6099. The examiner can normally be reached on 8:30AM-5:00PM.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran can be reached on (571) 272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Art Unit: 1631

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/ERIC S. DEJONG/
Primary Examiner, Art Unit 1631